A Spectral Approach to the Nonclassical Transport Equation (looking for better title)

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Abstract

These notes describe an approach to manipulate the nonclassical transport equation into a classical form that can be numerically solved through traditional approaches. The approach uses a combination of the spectral method and source iteration to eliminate the s-dependence. We use the LTS$_N$ method to solve the resulting equation in a 1-D system.

Keywords: tbd, tbd

0. Introduction

The theory of *nonclassical* particle transport, which describes processes in which a particle's distance-to-collision is *not* exponentially distributed, has received increased attention in the last decade. It was originally proposed by Larsen [1] to describe measurements of photon path-length in the Earth's cloudy atmosphere that could not be explained by classical radiative transfer (cf. [2]). The theory has been extended over the last few years [3–7] and has found applications in other areas, including neutron transport in certain types of nuclear reactors [8–10], computer graphics [11], and problems involving anomalous diffusion (cf. [12]). Moreover, a similar kinetic equation has been independently derived for the periodic Lorentz gas in a series of papers by Golse (cf. [13]) and by Marklof and Strömbergsson [14–17].

The nonclassical theory requires an extended phase space that includes an extra independent variable: the free-path s, representing the distance traveled by a particle since its previous interaction. The one-speed nonclassical transport equation can be written as [5]

$$\frac{\partial}{\partial s}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(\boldsymbol{\Omega},s)\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \tag{1a}$$

$$\delta(s)\left[c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')d\Omega' ds' + \frac{Q(\boldsymbol{x})}{4\pi}\right], \quad \boldsymbol{x}\in V,\ \boldsymbol{\Omega}\in 4\pi,\ 0<s,$$

where $\boldsymbol{x} = (x,y,z)$, $\boldsymbol{\Omega} = (\Omega_x,\Omega_y,\Omega_z)$, Ψ is the nonclassical angular flux, c is the scattering ratio, and Q is an isotropic source. Here, $P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})d\Omega$ represents the probability that when

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a particle with direction of flight $\mathbf{\Omega}'$ scatters, its outgoing direction of flight will lie in $d\Omega$ about $\mathbf{\Omega}$. This equation is subject to the incident boundary angular flux [18]

$$\Psi(\boldsymbol{x}, \mathbf{\Omega}, s) = \Psi^b(\boldsymbol{x}, \mathbf{\Omega})\delta(s), \quad \boldsymbol{x} \in \partial V, \ \boldsymbol{n} \cdot \mathbf{\Omega} < 0, \ 0 < s. \tag{1b}$$

The angular-dependent nonclassical total cross section $\Sigma_t(\mathbf{\Omega}, s)$ in Eq. (1a) satisfies

$$p(\mathbf{\Omega}, s) = \Sigma_t(\mathbf{\Omega}, s)e^{-\int_0^s \Sigma_t(\mathbf{\Omega}, s')ds'}, \tag{2}$$

where $p(\mathbf{\Omega}, s)$ is the free-path distribution function in the direction $\mathbf{\Omega}$.

If classical transport takes place, Σ_t is independent of both $\mathbf{\Omega}$ and s. In this case, the free-path distribution reduces to the exponential $p(s) = \Sigma_t e^{-\Sigma_t s}$, and Eqs. (1) reduce to the classical linear Boltzmann equation

$$\mathbf{\Omega} \cdot \nabla\Psi_c(\boldsymbol{x}, \mathbf{\Omega}) + \Sigma_t\Psi_c(\boldsymbol{x}, \mathbf{\Omega}) = c\int_{4\pi} P(\mathbf{\Omega}' \cdot \mathbf{\Omega})\Sigma_t\Psi_c(\boldsymbol{x}, \mathbf{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi}, \tag{3a}$$

$$\boldsymbol{x} \in V, \ \mathbf{\Omega} \in 4\pi,$$

$$\Psi_c(\boldsymbol{x}, \mathbf{\Omega}) = \Psi^b(\boldsymbol{x}, \mathbf{\Omega}), \quad \boldsymbol{x} \in \partial V, \ \boldsymbol{n} \cdot \mathbf{\Omega} < 0, \tag{3b}$$

for the classical angular flux

$$\Psi_c(\boldsymbol{x}, \mathbf{\Omega}) = \int_0^\infty \Psi(\boldsymbol{x}, \mathbf{\Omega}, s)ds. \tag{3c}$$

Numerical results for the nonclassical theory have been provided for diffusion-based approximations and for moment models in the diffusive regime [3, 8–10, 19, 20]. To our knowledge, numerical results for the nonclassical transport equation given by Eqs. (1) are only available for problems in rod geometry [21–23]. This is in part due to the difficult task of estimating the nonclassical free-path distribution. Another reason is that, given the s-dependence of Σ_t and the improper integral on the right-hand side of Eqs. (1), a direct deterministic approach that involves discretizing the variable s is inefficient.

The goal of this paper is to introduce an approach to numerically solve Eqs. (1) in a deterministic fashion, using available methods. We combine the multiple collision formalism [24] and a spectral approach to obtain a set of coupled differential equations that can be solved recursively. These equations have the form of a purely absorbing *classical* transport equation with a fixed (known) source, and can be solved by any traditional method. Here, we present numerical results to the one-dimensional (1-D) nonclassical transport equation in slab geometry under both classical and nonclassical assumptions. We use the LTS$_N$ method [25] to solve the set of classical equations. These results show ##### THAT EVERYTHING WORKS #####

The remainder of this paper is organized as follows. ##########

2. The Proposed Method (looking for better section title)

We consider Eq. (1a) in an equivalent "initial value" form:

$$\frac{\partial}{\partial s}\Psi(\boldsymbol{x}, \mathbf{\Omega}, s) + \mathbf{\Omega} \cdot \nabla\Psi(\boldsymbol{x}, \mathbf{\Omega}, s) + \Sigma_t(\mathbf{\Omega}, s)\Psi(\boldsymbol{x}, \mathbf{\Omega}, s) = 0, \tag{4a}$$

$$\Psi(\boldsymbol{x}, \mathbf{\Omega}, 0) = c\int_{4\pi}\int_0^\infty P(\mathbf{\Omega}' \cdot \mathbf{\Omega})\Sigma_t(\mathbf{\Omega}', s')\Psi(\boldsymbol{x}, \mathbf{\Omega}', s')d\Omega' ds' + \frac{Q(\boldsymbol{x})}{4\pi}, \tag{4b}$$

and define ψ such that

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) \equiv \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}. \tag{5}$$

We can now rewrite the nonclassical problem as

$$\frac{\partial}{\partial s}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega} \cdot \nabla \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = 0, \tag{6a}$$

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = S(\boldsymbol{x}, \boldsymbol{\Omega}) + \frac{Q(\boldsymbol{x})}{4\pi}, \tag{6b}$$

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \Psi^b(\boldsymbol{x}, \boldsymbol{\Omega})\delta(s) e^{\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}, \quad \boldsymbol{x} \in \partial V,\ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0, \tag{6c}$$

where

$$S(\boldsymbol{x}, \boldsymbol{\Omega}) = c \int_{4\pi} \int_0^\infty P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) p(\boldsymbol{\Omega}', s') \psi(\boldsymbol{x}, \boldsymbol{\Omega}', s') d\Omega' ds'. \tag{6d}$$

Using the theory of multiple collisions [24], we define

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \sum_{k=0}^{\infty} \psi^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}, s), \tag{7}$$

where $\psi^{(k)}$ represents the component of the angular flux consisting of particles that have undergone *exactly* k collisions. It is easy to see that $\psi^{(k)}$ satisfies

$$\frac{\partial}{\partial s}\psi^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega} \cdot \nabla \psi^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}, s) = 0, \quad k = 0, 1, 2, \dots, \tag{8a}$$

$$\psi^{(0)}(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = \frac{Q(\boldsymbol{x})}{4\pi}, \tag{8b}$$

$$\psi^{(0)}(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \Psi^b(\boldsymbol{x}, \boldsymbol{\Omega})\delta(s) e^{\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}, \quad \boldsymbol{x} \in \partial V,\ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0, \tag{8c}$$

$$\psi^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = S^{(k-1)}(\boldsymbol{x}, \boldsymbol{\Omega}), \quad k = 1, 2, \dots, \tag{8d}$$

$$\psi^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}, s) = 0, \quad \boldsymbol{x} \in \partial V,\ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0,\ k = 1, 2, \dots, \tag{8e}$$

where $S^{(k-1)}(\boldsymbol{x}, \boldsymbol{\Omega}) = c \int_{4\pi} \int_0^\infty P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) p(\boldsymbol{\Omega}', s') \psi^{(k-1)}(\boldsymbol{x}, \boldsymbol{\Omega}', s') d\Omega' ds'$.

To apply the spectral method, we approximate $\psi^{(k)}$ by a truncated series of Laguerre polynomials [26] in s:

$$\psi^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \sum_{m=0}^{M} \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) L_m(s), \quad k = 0, 1, 2, \dots, \tag{9}$$

and replace this ansatz into Eqs. (8). The Laguerre polynomials $\{L_0(s), L_1(s), \dots, L_M(s)\}$ are orthogonal with respect to the weight function e^{-s}, and satisfy $\frac{d}{ds}L_m(s) = \left(\frac{d}{ds} - 1\right) L_{m-1}(s)$ for $m > 0$. Therefore, multiplying Eqs. (8a), (8c) and (8e) by $e^{-s}L_m(s)$ and operating on them by $\int_0^\infty (\cdot) ds$, we obtain

$$\boldsymbol{\Omega} \cdot \nabla \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = \sum_{j=m+1}^{M} \psi_j^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}), \quad m = 0, 1, \dots, M,\ k = 0, 1, 2, \dots, \tag{10a}$$

$$\psi_m^{(0)}(\boldsymbol{x}, \boldsymbol{\Omega}) = \Psi^b(\boldsymbol{x}, \boldsymbol{\Omega}), \quad \boldsymbol{x} \in \partial V,\ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0,\ m = 0, 1, \dots, M, \tag{10b}$$

$$\psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = 0, \quad \boldsymbol{x} \in \partial V,\ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0,\ m = 0, 1, \dots, M,\ k = 1, 2, \dots. \tag{10c}$$

Moreover, Eqs. (8b) and (8d) respectively yield

$$\sum_{j=m+1}^{M} \psi_j^{(0)}(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{Q(\boldsymbol{x})}{4\pi} - \sum_{j=0}^{m} \psi_j^{(0)}(\boldsymbol{x},\boldsymbol{\Omega}), \tag{11a}$$

$$\sum_{j=m+1}^{M} \psi_j^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) = S^{(k-1)}(\boldsymbol{x},\boldsymbol{\Omega}) - \sum_{j=0}^{m} \psi_j^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}), \quad k = 1, 2, \dots . \tag{11b}$$

Next, we define $U_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega})$ as

$$U_0^{(0)}(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{Q(\boldsymbol{x})}{4\pi}, \tag{12a}$$

$$U_0^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) = S^{(k-1)}(\boldsymbol{x},\boldsymbol{\Omega}), \quad k = 1, 2, \dots , \tag{12b}$$

$$U_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) = U_{m-1}^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) - \psi_{m-1}^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}), \quad m = 1, ..., M, \ k = 0, 1, 2, \dots . \tag{12c}$$

Finally, using Eqs. (10) and (11) and Eqs. (12), we can rewrite the nonclassical problem as a set of coupled differential equations:

$$\boldsymbol{\Omega} \cdot \nabla \psi_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) + \psi_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) = U_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}), \quad m = 0, 1, ..., M, \ k = 0, 1, 2, \dots , \tag{13a}$$

$$\psi_m^{(0)}(\boldsymbol{x},\boldsymbol{\Omega}) = \Psi^b(\boldsymbol{x},\boldsymbol{\Omega}), \quad \boldsymbol{x} \in \partial V, \ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0, \quad m = 0, 1, ..., M, \tag{13b}$$

$$\psi_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) = 0, \quad \boldsymbol{x} \in \partial V, \ \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0, \ m = 0, 1, ..., M, \ k = 1, 2, \dots . \tag{13c}$$

Equations (13) can be solved recursively using any homogeneous solver. Starting at $k = 0$, each $\psi^{(k)}$ is attained as follows:

1. $m = 0$;
2. While $m < M$
   - 2.1. Solve Eqs. (13) for $\psi_m^{(k)}$, using the fact that $U_m^{(k)}$ is a known function given by Eqs. (12);
   - 2.2. $m = m + 1$;
3. Use Eq. (9) to obtain $\psi^{(k)}$;
4. Repeat for $k = k + 1$.

Using a stopping criterion for the k iterations, the nonclassical angular flux Ψ is recovered from Eqs. (5) and (7). Finally, the angular flux $\Psi_c(\boldsymbol{x},\boldsymbol{\Omega})$ is obtained using Eq. (3c).

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DISCUSSION: APPROXIMATIONS, SOLVERS, COMMENTS ON CONVERGENCE, ETC.

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NUMERICAL APPROACH WE WILL PRESENT; 1-D SLAB

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3. Validation with Classical Transport

WE SHOW RESULTS FOR 1-D SLAB (???AND 3D???) TEST PROBLEMS WITH CLASSICAL TRANSPORT

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5. Nonclassical Results

WE SHOW RESULTS FOR 1-D SLAB TEST PROBLEMS WITH NONCLASSICAL TRANSPORT – E.G., RANDOM PERIODIC

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6. Conclusion

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Comments (for our discussion)

- While we do not explicitly discretize s, the following takes place:
  - $\psi(x, \mu, s)$ is approximated by a truncated series of Laguerre polynomials in s
  - The integral in s described in Eqs. (6) will probably need to be performed numerically
  - At the end of the algorithm, we need to calculate

    $$\hat{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) ds = \int_0^\infty \left(e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s') ds'} \sum_{k=0}^{K} \sum_{m=0}^{M} \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) L_m(s) \right) ds,$$

    which will also need to be performed numerically
  - The LTS_N matrix should be simple and easy; since it's purely absorbing, A is a diagonal matrix $1/\mu_n$
- The convolution integrals in LTS_N will *probably* need to be solved numerically due to the recursiveness of the problem arising from the source term. **Is there a way to do that analitically?**
- Due to the source iteration approach, convergence will be slow as problems become more diffusive.
- It is not clear to me what will be the more time-consuming step. My guess is that the time to converge the source iteration will dominate in diffusive problems; for absorbing problems, I do not know.

- Nonclassical boundary conditions are tricky because of the $\delta(s)$. I *expect* the method here to work, but there may be convergence problems due to the Laguerre approximation/truncation. We'll need to test it for a few problems and see what we get; I'll work on figuring out the analytical convergence. Still regarding the boundary conditions, it is possible that the best solution will be using the *forward* nonclassical equation. That, however, is beyond the current scope.

- To validate the method, we will apply the algorithm to solve classical problems. In that case, $p(\mu, s) = \Sigma_t e^{-\Sigma_t s}$. This will also allow us to see how efficiently the method is.

- After it is validated, we can apply the algorithm to the random periodic case we have been working on; in the future, we can go for general stochastic mixtures.

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